

# Symmetry relations for spin-resolved exchange correlation kernels in soft magnetic layered systems

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We first exploit the physical condition satisfying the symmetry relation of the “exact” spin-resolved exchange correlation kernel based on the “mixed scheme” in soft magnetic layered systems. The conditions are derived and examined by taking into account the field gradients of the magnetic moment as well as that of the electric moment. We also exploit the physical condition by means of deviation distribution function suitable for complex electronic structures with arbitrary  $\zeta$ .

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Density functional theory (DFT) has been a chief support of the condensed matter theory for its practical prediction of various properties of many-electron system. It has resolved many properties such as the ground state energies, forces on the atoms or molecules, and their equilibrium positions [1]. Its local density approximations including density gradient corrections have generally been used for their simplicity and accuracy [1, 2]. Unfortunately, there have been some exceptions for their accuracy. On top of that, semilocal approximations fail to describe the long range interaction between electrons whose densities do not or weakly overlap. As an alternative, the “mixed scheme” has been proposed [3, 4, 5, 6, 7]. In this scheme, the Coulomb electron-electron interaction is decomposed into the short range (SR) part and the complementary long range (LR) part. The key concept is then to use a semilocal approximation for SR part and a more appropriate many-body methods for LR part.

In view of practical interests for spin transport properties of soft magnetic layered systems, the resolution of topics of the weak dispersion or van der Waals forces is clearly important. Additionally, there has been growing great deal of interests for the magnetic information storage system basically containing soft ferromagnets [8, 9, 10, 11]. These storage applications are based on the idea of the “spin-torque switching” in ferromagnetic-normal-ferromagnetic metal hybrid structures. The idea has been proposed by Slonczewski [12, 13] and Berger [14] as an attractive alternative of controlling the magnetization in place of the traditional way of modulating magnetic fields. Considerable evidence for the concept has been accumulated by demonstrating that the magnetization can be switched or precessed in a soft ferromagnet, because a current exerts “spin-transfer torque” on a thin free magnetic layer, which is polarized in a thick “fixed” magnetic layer [8, 9, 10, 11, 12, 13, 14]. Such interests inspired us to propose symmetry relations for the exchange correlation kernel (XCK) in soft magnetic systems involving intricate boundary conditions and corresponding spin scatterings.

As one of the central signatures in DFT, XCK can

be useful for giving direct insight into the dynamics of spin interactions in multilayer system. XCK is a basic concept in describing many body correlation effects in an inhomogeneous electron liquid and is a vital element of the spin susceptibility. Spin-resolved XCK  $f_{ss'}^{\text{xc}}(\zeta)$  is defined by

$$f_{ss'}^{\text{xc}}(\zeta) \equiv \frac{\partial^2 E^{\text{xc}}(\mathbf{r}, \mathbf{r}'; \zeta)}{\partial n_{s'}(\mathbf{r}) \partial n_s(\mathbf{r}')} \quad (1)$$

where  $E^{\text{xc}}$  is the total XC energy functional in many electron system with spin polarization  $\zeta$ . Here,  $n_s(n_{s'})$  denotes the electron density in spin state  $s(s')$ .  $f_{ss'}^{\text{xc}}(\zeta)$  satisfies the symmetry relation

$$f_{\bar{s}\bar{s}}^{\text{xc}}(\zeta) = f_{\bar{s}\bar{s}}^{\text{xc}}(-\zeta) \quad (2)$$

which is a key property of XCK and equally a fundamental idea of importance in condensed matter. The specific symmetry relation

$$f_{\bar{s}\bar{s}}^{\text{xc}}(\zeta) = f_{\bar{s}\bar{s}}^{\text{xc}}(\zeta) \quad (3)$$

also plays a significant role to investigate the situations in artificial composite structures [15]. However, prior to our previous work, there was no attempt to interpret XCK in terms of directly measurable quantities such as spin current  $I_{s(\bar{s})}$ . Although considerable studies have been devoted to investigate  $I_{s(\bar{s})}$ , theoretical approaches have substantially been limited to oversimplified multilayer systems unsuitable for more realistic applications.

The introduced key idea in this letter is the accurate relations guaranteeing the specific symmetry relation in soft magnetic layered systems. The accurate relations are derived explicitly by including not only the field gradient of the electric moment but also that of the magnetic moment. We also explicitly show the relation which guarantees the specific symmetry relation by using the solution of Boltzmann equation without neglecting anisotropic terms in systems of various dimensions. The condition satisfying the specific symmetry relation could be related to the spin density variation  $\nabla n_{s(\bar{s})}$  and

then  $\nabla n_{s(\bar{s})}$  to the variation of electrochemical potential  $\nabla \mu_{s(\bar{s})}$ . Hence a general inhomogeneous multilayer system with arbitrary magnetization alignments can be explored easily by examining properties of XCK on the basis of  $I_{s(\bar{s})} \propto -\frac{\partial \mu_{s(\bar{s})}}{\partial x}$ .

Density functional based on the “mixed scheme” is given by the sum of the kinetic energy  $T$  of a noninteracting particle system, SR and LR potential energies  $U(\equiv U_S + U_L)$ , and unknown SR and LR functionals  $E^{\text{xc}}(\equiv E_S^{\text{xc}} + E_L^{\text{xc}})$ ;  $E[n(\mathbf{r})] = T[n(\mathbf{r})] + U[n(\mathbf{r})] + E^{\text{xc}}$  in terms of one particle density in N-electron system

$$n(\mathbf{r}) = N \sum_{s_2, \dots, s_N} \int |\Psi(\mathbf{r}s, \mathbf{r}_2 s_2 \dots, \mathbf{r}_N s_N)|^2 d\mathbf{r}_2, \dots, d\mathbf{r}_N.$$

Once SR (LR) part is given by  $T[n(\mathbf{r})] + U_{S(L)}[n(\mathbf{r})] + E_S^{\text{xc}}$ , the complementary LR (SR) part is the difference between the universal functional  $E[n(\mathbf{r})]$  and the SR (LR) part. In pair density theory giving a more improved ground state energy than in one particle density [7], the spin-summed pair density is given by  $n(\mathbf{r}_1, \mathbf{r}_2) = \frac{N(N-1)}{2} \sum_{s_1 s_2} \gamma_{s_1 s_2}(\mathbf{r}_1, \mathbf{r}_2)$  where  $\gamma_{s_1 s_2}(\mathbf{r}_1, \mathbf{r}_2)$  is the spin-resolved diagonal of the two-body reduced density matrix [6]. The exact energy density functional is given by  $E[n(\vec{x})] = T[n(\vec{x})] + U$  with  $\vec{x} = (\mathbf{r}_1, \mathbf{r}_2)$ . Here,  $U(\equiv U_S + U_L)$  consists of the external potential of a given pair and the interaction potential between particles forming two pairs at  $\vec{x}_i = (\mathbf{r}_{i1}, \mathbf{r}_{i2})$  and  $\vec{x}_j = (\mathbf{r}_{j1}, \mathbf{r}_{j2})$  [7]. Hence, the total XC energy functional  $E^{\text{xc}}$  in an interacting system can be described in terms of pair density  $n(\vec{x})$

$$E^{\text{xc}}[n(\mathbf{r})] = T[n(\vec{x})] - T[n(\mathbf{r})] + U[n(\vec{x})] - U[n(\mathbf{r})].$$

$E^{\text{xc}}$  contains the unknown remaining kinetic term  $\Delta T \equiv T[n(\vec{x})] - T[n(\mathbf{r})]$  as well as the interparticle interaction potential. Here,  $\Delta T$  denotes the difference between the exact kinetic term  $T[n(\vec{x})]$  in an interacting scheme and noninteracting counter part  $T[n(\mathbf{r})]$ .  $f_{s\bar{s}}^{\text{xc}}$ , the second derivatives of  $E^{\text{xc}}$  with respect to spin densities  $n_s(\mathbf{r})$  and  $n_{\bar{s}}(\mathbf{r}')$  at a given pair position  $\vec{x}_i = (\mathbf{r}, \mathbf{r}')$ , is now written in the form

$$f_{s\bar{s}}^{\text{xc}}(\zeta) = \frac{\nabla_{\mathbf{r}} \nabla_{\mathbf{r}'} [\Delta T[n(\vec{x})] + U[n(\vec{x})] - U[n(\mathbf{r})]]}{\nabla n_{\bar{s}}(\mathbf{r}) \nabla n_s(\mathbf{r}')} \quad (4)$$

For the defined XCK by Eq.(1), the symmetry relation  $f_{s\bar{s}}^{\text{xc}}(\zeta) = f_{\bar{s}s}^{\text{xc}}(-\zeta)$  is trivial in an inhomogeneous system of broken spin symmetry since majority and minority spins interchange their orientations and positions with the reversed polarization  $-\zeta$ . That is, based on the assumption that the physical condition

$$\frac{\nabla n_{\bar{s}}(\mathbf{r}')}{\nabla n_s(\mathbf{r}')} = \frac{\nabla n_{\bar{s}}(\mathbf{r})}{\nabla n_s(\mathbf{r})} \quad (5)$$

is fulfilled (i.e., the ratios of spin density gradients are the same at two different positions  $\mathbf{r}$  and  $\mathbf{r}'$ ), the specific

symmetry relation

$$f_{s\bar{s}}^{\text{xc}}(\zeta) = \frac{\partial^2 E^{\text{xc}}(\mathbf{r}, \mathbf{r}'; \zeta)}{\partial n_{\bar{s}}(\mathbf{r}) \partial n_s(\mathbf{r}')} = \frac{\partial^2 E^{\text{xc}}(\mathbf{r}, \mathbf{r}'; \zeta)}{\partial n_s(\mathbf{r}) \partial n_{\bar{s}}(\mathbf{r}')} = f_{\bar{s}s}^{\text{xc}}(\zeta) \quad (6)$$

is obtained trivially. So to speak, we explicitly show the specific symmetry relation by using XCK defined on the “mixed scheme”. Hence it is elucidated that Eqs.(5) and (6) can be used to investigate soft magnetic systems without difficulty. Equation(5) thus can be useful to examine the adequacy of the specific symmetry relation in particular for the present weakly interacting systems.

The continuity equation for the probability density  $\rho_{\mathbf{M}}(t) [\equiv \mu_B(n_s - n_{\bar{s}})]$  is written in form [16]

$$\frac{\partial \rho_{\mathbf{M}}(t)}{\partial t} = -\nabla \cdot \mathbf{j}_{\mathbf{M}}(t) \quad (7)$$

where the probability current density  $\mathbf{j}_{\mathbf{M}}(t) [\equiv \mu_B(\mathbf{j}_s - \mathbf{j}_{\bar{s}})]$  on  $\mathbf{M}$ -sphere is given by [9]

$$\mathbf{j}_{\mathbf{M}}(t) = \rho_{\mathbf{M}}(t) \dot{\mathbf{M}}_{\text{det}} - D \nabla \rho_{\mathbf{M}}(t) \quad (8)$$

where  $D$  is the diffusion constant in the case that diffusion constants of up-spin and down-spin are the same. Here,  $\dot{\mathbf{M}}_{\text{det}}$  is the deterministic part of the Landau-Lifshitz (LL) equation for the evolution of a uniform magnetization  $\mathbf{M}(t)$ . The deterministic part is the sum of the conservative precession, dissipative LL damping, Slonczewski current-induced term [9], and a neglected term in the current-induced part [8];

$$\begin{aligned} \dot{\mathbf{M}}_{\text{det}} = & -\gamma \mathbf{M} \times \mathbf{H}_{\text{cons}} - \gamma \alpha M \hat{m} \times (\hat{m} \times \mathbf{H}_{\text{cons}}) \\ & -\gamma J M \hat{m} \times (\hat{m} \times \hat{m}_p) - \frac{\gamma \hbar \tilde{g}^{s\bar{s}}}{8\pi M} \hat{m} \times \frac{d\hat{m}}{dt} \end{aligned} \quad (9)$$

where  $\gamma$ ,  $M$ ,  $\alpha$ , and  $J$  are, respectively, the gyromagnetic ratio, saturation magnetization, LL damping constant, and an empirical constant with units of magnetic field which is proportional to the current. Here,  $\hat{m} \equiv \mathbf{M}/M$  and  $\hat{m}_p$  is the unit vector along the magnetization and the easy axis. In the first and second terms,  $\mathbf{H}_{\text{cons}}$  is the field around which  $\mathbf{M}$  precesses as conservative and is related with the magnetic energy  $E_{\mathbf{M}}$  via  $\mu_0 \mathbf{H}_{\text{cons}} = -\frac{\partial E_{\mathbf{M}}}{\partial \mathbf{m}}$ . The magnetic energy  $E_{\mathbf{M}}$  is the sum of the anisotropy energy and the coupling term with an external field [9]. When the last term (containing the mixing conductance  $\tilde{g}^{s\bar{s}}$ ) is neglected, the current-induced part in Eq.(9) is consistent with the result of Slonczewski [8].

The current for up (down)-spin carriers can be written by

$$\mathbf{j}_{s(\bar{s})} = -n_{s(\bar{s})} \nu \mathbf{E} \pm n_{s(\bar{s})} \frac{\dot{\mathbf{M}}_{\text{det}}}{2} - D_{s(\bar{s})} \nabla n_{s(\bar{s})} \quad (10)$$

where  $\nu$  is the mobility and  $D_{s(\bar{s})}$  is the spin-up (down) diffusion constant. Equation(10) is based on the fact that the drift velocity is proportional to the force on

the conduction electron. The force originates from the field gradients of its electric and magnetic moment (i.e.,  $\kappa \mathbf{v}_s = \mathbf{F}_s = -e\mathbf{E} \pm \mu_B \nabla H_{\text{eff}}$ ) [10]. Here, the effective field  $H_{\text{eff}}$  includes the external field and the molecular field coupled to the conduction electron via an exchange constant. Hence, the spin-up (down) velocity  $v_{s(\bar{s})} = -\nu \mathbf{E} \pm \mathbf{M}_{\text{det}}/2$  is applied in Eq.(10), because the difference between the velocities of up-spin and down-spin is given by  $v_s - v_{\bar{s}} = 2\mu_B \nabla H_{\text{eff}}/\kappa = \mathbf{M}_{\text{det}}$  from Eq.(8)

The probability density  $\rho_{\mathbf{M}}$  often depends only on energy, for instance, in a thermal equilibrium or a nonequilibrium steady state without LL damping  $\alpha$  and current  $J$ . For this reason, the density  $\rho_{\mathbf{M}}(t)$  can be replaced with  $\rho_{\mathbf{M}}(\varepsilon, t)$  from the assumption that  $\rho_{\mathbf{M}}(\varepsilon, t)$  depends only on energy. Still energy dependence can be different in distinct positions of sphere. Together with  $\rho_{\mathbf{M}}(\varepsilon, t)$ , the spin-up (down) probability current density can be obtained by

$$\begin{aligned} j_{s(\bar{s})}(\varepsilon, t) &= \oint [\mathbf{j}_{s(\bar{s})} \times d\mathbf{M}] \cdot \hat{\mathbf{m}} \\ &= n_{s(\bar{s})}(\varepsilon, t) \left\{ \nu I^{\text{EE}} \mp \frac{\gamma}{2} \left[ (\alpha M - \frac{\gamma \hbar \tilde{g}^{s\bar{s}}}{8\pi}) I^{\text{HE}} - J \hat{\mathbf{m}}_p \cdot I^{\text{M}} \right] \right\} \\ &\quad - D_{s(\bar{s})} \frac{\partial n_{s(\bar{s})}(\varepsilon, t)}{\partial \varepsilon} \mu_0 I^{\text{HE}}. \end{aligned} \quad (11)$$

Here, energy integrals for the electric field  $I^{\text{EE}}$  and the magnetic field  $I^{\text{HE}}$ , and magnetization integral  $I^{\text{M}}$  are defined, respectively, by

$$\begin{aligned} I^{\text{EE}} &\equiv \oint d\mathbf{M} \times \mathbf{E} \cdot \hat{\mathbf{m}} \\ I^{\text{HE}} &\equiv \oint d\mathbf{M} \times \mathbf{H}_{\text{cons}} \cdot \hat{\mathbf{m}} = \oint H_{\text{cons}} dM \\ I^{\text{M}} &\equiv \oint d\mathbf{M} \times \mathbf{M} \cdot \hat{\mathbf{m}}. \end{aligned} \quad (12)$$

On the assumption that the system is in steady state, the probability current density  $\mathbf{j}_{\mathbf{M}}(t)$  vanishes. To get some insight in Eq.(11), we consider possible systems in steady state (i.e.,  $\mathbf{j}_{\mathbf{M}}(t) = 0$ ) and investigate the specific symmetry relation in each feasible case. A steady state is reached if the condition  $j_s(\varepsilon) = j_{\bar{s}}(\varepsilon)$  is satisfied. After some straight forward algebra, we can write the relation corresponding to above condition  $j_s(\varepsilon) = j_{\bar{s}}(\varepsilon)$  by

$$\begin{aligned} \mu_0 I^{\text{HE}} \left( \frac{D_s \nabla n_s - D_{\bar{s}} \nabla n_{\bar{s}}}{\nabla \varepsilon} \right) &= \nu I^{\text{EE}} (n_s(\varepsilon) - n_{\bar{s}}(\varepsilon)) \\ - \frac{\gamma}{2} \left[ (\alpha M - \frac{\gamma \hbar \tilde{g}^{s\bar{s}}}{8\pi}) I^{\text{HE}} - J \hat{\mathbf{m}}_p \cdot I^{\text{M}} \right] &= (n_s(\varepsilon) + n_{\bar{s}}(\varepsilon)) \end{aligned} \quad (13)$$

Equation (13) leads us to following feasible situations in the system. First consider the case that up-spin and down-spin densities are the same. As long as the ratio of the work of the current induced torque to that of the LL damping  $\hat{\mathbf{m}}_p \cdot I^{\text{M}}/I^{\text{HE}}$  is equal to  $(\alpha M - \frac{\gamma \hbar \tilde{g}^{s\bar{s}}}{8\pi})/J$

and  $I^{\text{HE}} \neq 0$ , the condition which guarantees the specific symmetry relation is

$$\left. \frac{\nabla n_s}{\nabla n_{\bar{s}}} \right|_r = \left. \frac{\nabla n_s}{\nabla n_{\bar{s}}} \right|_{r'} = \frac{D_s}{D_{\bar{s}}}. \quad (14)$$

In this situation, the specific symmetry relation is trivially satisfied in normal region due to  $D_s = D_{\bar{s}}$ . Another possible meaningful situation satisfying  $j_s(\varepsilon) = j_{\bar{s}}(\varepsilon)$  is that  $n_s + n_{\bar{s}} = 0$  resulted in  $\nabla n_s + \nabla n_{\bar{s}} = 0$ . As long as  $\nu I^{\text{EE}} = 0$  and  $I^{\text{HE}} = 0$ , the condition assuring the specific symmetry relation is given by

$$\left. \frac{\nabla n_s}{\nabla n_{\bar{s}}} \right|_r = \left. \frac{\nabla n_s}{\nabla n_{\bar{s}}} \right|_{r'} = -1. \quad (15)$$

In this case, Eq.(15) is in agreement with the previous condition [15] for the specific symmetry relation in non-metallic region of a homogeneous system with no space charge. Even though the term containing the mixing conductance  $\tilde{g}^{s\bar{s}}$  in Eq.(9) is neglected as the case of Slonczewski [8], all the situations examined here satisfy the same conditions, Eqs.(14) and (15), assuring the specific symmetry relation in the similar way with no terms of  $\tilde{g}^{s\bar{s}}$ . As ever, these results are very useful to investigate spin related phenomena particularly in the normal metal region between two ferromagnets due to the condition  $D_s = D_{\bar{s}}$ .

Regarding realistic systems such as quasi-two or three dimensional multilayer and complicated electronic structures, corresponding spin-dependent scattering need to be considered. Consequently, the neglected anisotropic terms and coordinate variables [19, 20] have to be considered in electron distribution functions. For this purpose, we examine the spin current density given by [17]

$$\mathbf{j}_{s(\bar{s})} = -e \left( \frac{m}{\hbar} \right)^3 \int d^3 v v g_{\mathbf{v}}^{s(\bar{s})}(\varepsilon, \mathbf{r}) \quad (16)$$

in terms of deviation distribution function  $g_{\mathbf{v}}^{s(\bar{s})}(\varepsilon, \mathbf{r})$  corresponding to the energy  $\varepsilon$  and velocity  $v$ . A possible solution is given by

$$g_{\mathbf{v}}^{s(\bar{s})}(\varepsilon, \mathbf{r}) = e \mathbf{E} \frac{\partial f_0(\varepsilon)}{\partial \varepsilon} \lambda_{\text{eff}}^{s(\bar{s})}(\hat{\mathbf{v}}, \mathbf{r}) \quad (17)$$

for a system with all diffusive boundary effects driven by an applied electric field. It is valid in systems of various dimensions without neglecting anisotropic terms. Here, the effective mean free path is given by [17]  $\lambda_{\text{eff}}^{s(\bar{s})}(\vartheta, \mathbf{r}) = \lambda^{s(\bar{s})}(\vartheta) \left[ 1 - \exp\left(\frac{-|\mathbf{r}_0 - \mathbf{r}|}{\lambda^{s(\bar{s})}(\vartheta)}\right) \right]$  corresponding to an electron with normalized velocity  $\hat{\mathbf{v}}$  passing through a position  $\mathbf{r}$  in the direction  $\mathbf{r}_0 - \mathbf{r}$  with  $\mathbf{r}_0$  on the cylindrical boundary. The intrinsically anisotropic mean free path  $\lambda^{s(\bar{s})}(\vartheta)$  is given by  $\lambda_0^{s(\bar{s})} [1 - a^{s(\bar{s})} \cos^2 \vartheta - b^{s(\bar{s})} \cos^4 \vartheta]$  where  $\vartheta$  is the angle between the magnetization  $\mathbf{M}$  and velocity  $\mathbf{v}$ . When we compare Eq.(17) with another solution [18],

$$\hat{\mathbf{v}} \cdot e \mathbf{E} \lambda_{\text{eff}}^{s(\bar{s})}(\vartheta, \mathbf{r}) = \bar{\mu} - \mu^{s(\bar{s})}(\mathbf{r}) + \hat{\mathbf{v}} \cdot e \mathbf{E} \lambda_0^{s(\bar{s})} \quad (18)$$

where  $\bar{\mu}$  is the equilibrium electrochemical potential. Accordingly, the relation convincing the specific symmetry relation is given by

$$\frac{N_s(\varepsilon_F)}{N_{\bar{s}}(\varepsilon_F)} \frac{\nabla \{ \hat{v} \cdot e\mathbf{E} [1 - \lambda_{\text{eff}}^s(\vartheta, \mathbf{r})] \} - e\mathbf{E}}{\nabla \{ \hat{v} \cdot e\mathbf{E} [1 - \lambda_{\text{eff}}^{\bar{s}}(\vartheta, \mathbf{r})] \} - e\mathbf{E}} \bigg|_{\mathbf{r}} = \frac{\nabla n_s}{\nabla n_{\bar{s}}} \bigg|_{\mathbf{r}}. \quad (19)$$

Equation(19) is based on the relation given, in the presence of an electric field ( $\mathbf{E} = -\nabla\Phi$ ), by [20]

$$\nabla n_{s(\bar{s})} = eN_{s(\bar{s})}(\varepsilon_F)[\nabla\mu_{s(\bar{s})} - e\mathbf{E}].$$

Here  $N_{s(\bar{s})}(\varepsilon_F)$  is the spin-up (down) density of states at the Fermi level in a highly degenerate system. In order to generalize Eq.(19), we compare  $g_v^{s(\bar{s})}(\varepsilon, \mathbf{r})$  given by Eq.(18) with another solution [21] obtained by using the path integral along  $\mathbf{v}$ . The gradient of the electrochemical potential is then obtained by

$$\begin{aligned} \nabla\mu_{s(\bar{s})}(\mathbf{r}) = & -\nabla[\hat{S}_{s(\bar{s})\beta}(\mathbf{r}, \mathbf{r}')\hat{g}_{\beta\gamma}(\mathbf{v}, \mathbf{r}')\hat{S}_{\gamma s(\bar{s})}^\dagger(\mathbf{r}, \mathbf{r}')] \\ & -\nabla \int_{\Gamma(\mathbf{r}, \mathbf{r}')} dl'' \hat{S}_{s(\bar{s})\beta}(\mathbf{r}, \mathbf{r}'')\hat{v} \cdot e\mathbf{E}(\mathbf{r}'')\hat{S}_{\gamma s(\bar{s})}^\dagger(\mathbf{r}, \mathbf{r}'') \frac{\partial f_0}{\partial \varepsilon} \\ & +\nabla(\hat{v} \cdot e\mathbf{E}\lambda_0^{s(\bar{s})}) \end{aligned} \quad (20)$$

where the spinor propagation factor is given by  $\hat{S}(\mathbf{r}, \mathbf{r}') = P_{\mathbf{r}' \rightarrow \mathbf{r}} \exp(-\frac{1}{2} \int_{\Gamma(\mathbf{r}, \mathbf{r}')} dl'' \hat{\xi}(\mathbf{r}''))$  with the inverse mean-free path operator  $\hat{\xi}(\mathbf{r}'')$ . Here,  $P_{\mathbf{r}' \rightarrow \mathbf{r}}$  is the path ordering operator along  $\Gamma(\mathbf{r}, \mathbf{r}')$  which stands for the oriented straight path that starts at point  $\mathbf{r}'$  and ends up at  $\mathbf{r}$ . If we take the limiting case of sufficiently large value of  $|\mathbf{r} - \mathbf{r}'|$ , Eq.(20) is written by

$$\begin{aligned} \nabla\mu_{s(\bar{s})}(\mathbf{r}) = & -\nabla \int_{\Gamma(\mathbf{r}, \mathbf{r}')} dl'' [\hat{S}_{s(\bar{s})\beta}(\mathbf{r}, \mathbf{r}'')\hat{v} \cdot e\mathbf{E}(\mathbf{r}'') \\ & \hat{S}_{\gamma s(\bar{s})}^\dagger(\mathbf{r}, \mathbf{r}'') \frac{\partial f_0}{\partial \varepsilon}] + \nabla(\hat{v} \cdot e\mathbf{E}\lambda_0^{s(\bar{s})}). \end{aligned} \quad (21)$$

The first term on the right hand side in Eq.(21) corresponds to  $-\nabla(\hat{v} \cdot e\mathbf{E}\lambda_{\text{eff}}^{s(\bar{s})}(\hat{\mathbf{v}}, \mathbf{r}))$  in Eq.(19) assuring the specific symmetry relation. Hence the condition assuring the symmetry relation is written by

$$\frac{N_s(\varepsilon_F)}{N_{\bar{s}}(\varepsilon_F)} \frac{\nabla[\hat{v} \cdot e\mathbf{E}\lambda_0^s - \int_{\Gamma(\mathbf{r}, \mathbf{r}')} dl'' \hat{S}_{s\beta}(\mathbf{r}, \mathbf{r}'')\hat{v} \cdot e\mathbf{E}(\mathbf{r}'')\hat{S}_{\gamma s}^\dagger(\mathbf{r}, \mathbf{r}'') \frac{\partial f_0}{\partial \varepsilon}] - e\mathbf{E}}{\nabla[\hat{v} \cdot e\mathbf{E}\lambda_0^{\bar{s}} - \int_{\Gamma(\mathbf{r}, \mathbf{r}')} dl'' \hat{S}_{\bar{s}\beta}(\mathbf{r}, \mathbf{r}'')\hat{v} \cdot e\mathbf{E}(\mathbf{r}'')\hat{S}_{\gamma \bar{s}}^\dagger(\mathbf{r}, \mathbf{r}'') \frac{\partial f_0}{\partial \varepsilon}] - e\mathbf{E}} \bigg|_{\mathbf{r}} = \frac{\nabla n_s}{\nabla n_{\bar{s}}} \bigg|_{\mathbf{r}},$$

Hence, Eq.(19) and above related condition can be used to account adequately for experimental results. Once some quantities such as  $\mathbf{v}$ ,  $\mathbf{E}$  and the angle  $\vartheta$  at distinct positions are known, we can check the properties of XCK with ease. Besides, we can determine the relevance of theoretical and experimental consequences, particularly in the region satisfying the specific symmetry relation such as a homogeneous nonmagnetic system. For example, in case of choosing correct factors except an inappropriate  $\lambda_{\text{eff}}^{s(\bar{s})}$ , Eq.(19) is not satisfied in trivial

situations and proper modification for components such as  $a^{s(\bar{s})}$  and  $b^{s(\bar{s})}$  of  $\lambda_{\text{eff}}^{s(\bar{s})}$  would be done to be in agreement with the relation. Also experimental values can be investigated as well and be compared with the modified calculations.

Here, we have shown the conditions confirming the specific symmetry relation in current soft magnetic layered systems. First, the specific symmetry relation has been elaborated by defining XCK explicitly on the “mixed scheme” compared with our pervious work [15]. Then the conditions are derived by taking into account the field gradients of the magnetic moment in addition to that of the electric moment. At the same time, special attention is paid to the fact that when we consider the neglected anisotropic term in Boltzmann equation, it gives deviation from generally accepted definition of the electrochemical potential. For the first time, we have thus given the physical condition by dealing with deviation distribution function suitable for complex electronic structures in addition to one dimensional systems.

In conclusion, we have proposed a new method to confirm the relevance of studies of the spin-related phenomena in soft magnetic layered systems of various dimensions by taking the physical condition  $\frac{\nabla n_{\bar{s}}}{\nabla n_s} \big|_{\mathbf{r}} = \frac{\nabla n_{\bar{s}}}{\nabla n_s} \big|_{\mathbf{r}'}$  into account. Once some quantities in the condition are given, the properties of XCK can easily be checked theoretically and experimentally particularly in the region where the situation for convincing the specific symmetry relation is known. Furthermore, excellent agreement of theoretical and experimental results can be induced by modifying factors or experimental conditions in accord with the physical condition.

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